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Symmetry restoration in the mean-field description of proton-neutron pairing

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ABSTRACT

We show that the symmetry-restored paired mean-field states (quasiparticle vacua) properly account for isoscalar versus isovector nuclear pairing properties. Full particle-number, spin, and isospin symmetries are restored in a simple SO(8) proton-neutron pairing model, and prospects to implement a similar approach in a realistic setting are delineated. Our results show that, provided all symmetries are restored, the pictures based on pair-condensate and quartet-condensate wave functions represent equivalent ways of looking at the physics of nuclear proton-neutron pairing.

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A key question in nuclear structure physics is do proton-neutron (pn) pairs form collective condensates in nuclei in the same way that like-particle pairs do? Ever since the existence of like-particle nuclear pairing was suggested in 1958 by Bohr, Motelson, and Pines [1], this simple question has been addressed in numerous studies [2]. As late as in 2004, the authors of Ref. [3] concluded that *in spite of many attempts to extend the quasiparticle approach to incorporate the effect of pn correlations, no symmetry-unrestricted mean-field calculations of pn pairing, based on realistic effective interaction and the isospin conserving formalism have been carried out.* This conclusion still holds even today.

In this Letter, we show that sometimes contradicting conclusions about the existence of the pn pair condensate may have resulted from using a mean-field formalism without full symmetry restoration. Here we apply this formalism within simultaneous breaking and then restoration of three major symmetries: particle-number, angular-momentum, and isospin. In the shell-model framework these symmetries are not broken and hence do not have to be restored. A number of such studies already exist, see, e.g., Ref. [4]. However, the shell-model interprets the pn pairing as an effect of a strong nucleon-nucleon isoscalar interaction,

and is less concerned with the analysis of wave functions in terms of collective condensates. In this sense, the question of existence of the putative pn condensate remains open.

Due to the attractive nature of the nuclear interaction, atomic nuclei are strongly correlated systems exhibiting superfluid properties. The theoretical description of nuclear superfluidity is directly related to the theory of electronic superconductivity, wherein Cooper pairs of electrons in time-reversed states condensate near the Fermi level. In the nuclear case, we may expect a possible formation of six types of pairs, corresponding to the four degrees of freedom of the nucleon: spin and isospin, up and down. More precisely, we may have scalar-isovector Cooper pairs \hat{P}_v^+ , with three projections of the total isospin $v \equiv T_z=0, \pm 1$, and vector-isoscalar pairs \hat{D}_μ^+ , with three projections of the total spin $\mu \equiv S_z=0, \pm 1$. The condensation of spin-aligned \hat{D}_μ^+ pairs has recently attracted increased attention, see Refs. [5,6] and references cited therein.

The most general pair condensate is represented by a quasiparticle vacuum. This can be written in terms of the Thouless state [7, 8], which may be expressed as $|\Phi\rangle = \mathcal{N} \exp\{\hat{Z}^+\}|0\rangle$, for the Thouless pair \hat{Z}^+ given by

$$\hat{Z}^+ = \sum_{v=0,\pm 1} p_v \hat{P}_v^+ + \sum_{\mu=0,\pm 1} d_\mu \hat{D}_\mu^+. \quad (1)$$

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In the above equation, p_v and d_v are complex isovector and isoscalar amplitudes, respectively, $|0\rangle$ is the particle vacuum and \mathcal{N} is the normalization constant.

It is now obvious that in the Thouless state all symmetries: particle-number, spin, and isospin, are strongly mixed. Therefore, the standard paired-mean-field minimization of the average energy, which in nuclear physics is called Hartree-Fock-Bogolyubov (HFB) theory [8], may or may not give the best result. A great number of studies based on the HFB approach already exist, see, e.g., Refs. [9–13] and reviews in Refs. [2,3]. In this Letter, we argue that in order to analyze the problem of the pn pairing it is necessary to employ a more sophisticated approach that is based on the minimization of energy after all symmetries are restored.

The relevant method corresponds to the so-called variation-after-projection (VAP) [8] method, which employs the projected Thouless states,

$$|\Phi_{MK,NL}^{AST}\rangle = \hat{P}_A \hat{P}_{MK}^S \hat{P}_{NL}^T |\Phi\rangle, \quad (2)$$

as variational trial states. The projection operators: \hat{P}_A on particle number A , \hat{P}_{MK}^S on total spin S and its projection M , and \hat{P}_{NL}^T on total isospin T and its projection N , involve one-dimensional integration over the gauge angle, three-dimensional integration over the spin-rotation Euler angles and three-dimensional integration over the isospin-rotation Euler angles [8,14], respectively. In this Letter, we report on the implementation of a complete seven-dimensional integration which allows us to fully restore all relevant symmetries that are broken in an arbitrary symmetry-unrestricted Thouless state. Although such a technology has already been previously applied in the shell-model context [15], below we argue that it is essential for analyzing the physics of pn pairing.

However, before embarking on full-scale VAP calculations in a realistic nuclear DFT setting, one would like to know if such a complete and demanding approach is capable of bringing better solutions when applied in a simple model. For that, in this Letter we perform a full VAP analysis of the well-known SO(8) model [2, 16–21]. To make the properties of the model as clear as possible, we begin by a novel discussion of its building blocks and symmetries, and later we recall its Hamiltonian and dynamics.

The building blocks of the model are the isovector and isoscalar pairs within a single-particle phase space of a few degenerate ℓ shells,

$$\hat{P}_v^+ = \sum_{\ell} \sqrt{\frac{2\ell+1}{2}} \left(a_{\ell\frac{1}{2}\frac{1}{2}}^+ a_{\ell\frac{1}{2}\frac{1}{2}}^+ \right)_{M=0, S_z=0, T_z=v}^{L=0, S=0, T=1}, \quad (3)$$

$$\hat{D}_{\mu}^+ = \sum_{\ell} \sqrt{\frac{2\ell+1}{2}} \left(a_{\ell\frac{1}{2}\frac{1}{2}}^+ a_{\ell\frac{1}{2}\frac{1}{2}}^+ \right)_{M=0, S_z=\mu, T_z=0}^{L=0, S=1, T=0}, \quad (4)$$

where $a_{\ell\frac{1}{2}\frac{1}{2}}^+$ are the creation operators of a particle with orbital angular momentum ℓ , spin $\frac{1}{2}$, and isospin $\frac{1}{2}$. The round brackets denote triple standard Clebsch-Gordan coupling to the total orbital angular momentum L , spin S , and isospin T , having, respectively, projections M , S_z , and T_z . The maximum number of particles allowed in this phase space is equal to 4Ω for $\Omega = \sum_{\ell} (2\ell + 1)$. For deformed nuclei with spin-orbit coupling taken into account, the notion of spin should, in fact, be understood as that of the alispin [22], which pertains to a pair of deformed Kramers-degenerate single-particle states.

In the past, much of the discussion related to properties of pn pairing concentrated on the question of whether real or complex quasiparticle amplitudes have to be used. In order to solve this problem in the context of the most general Thouless pairs, defined

in Eq. (1), we briefly touch upon their symmetries. To begin, let us consider a system described by a scalar and isoscalar Hamiltonian, such as that in the SO(8) model, which is defined below.

In the first instance, we note that unabridged spin and isospin projections involve rotating the Thouless pair over the full spin and isospin SO(3) groups, hence, we can freely choose its initial orientations in the spin and isospin spaces, respectively. This means that the vector and isovector pair-creation operators, Eqs. (4) and (3), can be arbitrarily aligned along one of the directions in space and isospace, respectively. Without any loss of generality, we can choose orientations along the z axes, that is, we can keep in Eq. (1) only spherical amplitudes p_0 and d_0 . Then, the Thouless states become eigenstates of spin and isospin projections with $S_z = T_z = 0$. Such a choice has an enormous advantage, namely, it allows for reducing the integrations over the spin and isospin Euler angles to one dimension only, which reduces seven dimensions of integration to just three. We have also been able to test and benchmark all of our results by performing unrestricted integrations.

Second, we note that by a simple expansion of the exponential function, the particle-number projection of the Thouless state $|\Phi\rangle = \mathcal{N} \exp\{\hat{Z}^+\}|0\rangle$ is equal to $|\Phi_A\rangle = \mathcal{N}' (\hat{Z}^+)^{A/2} |0\rangle$ for $\mathcal{N}' = \mathcal{N}'(A/2)!$. Therefore, an overall multiplicative factor of the Thouless pair, and its phase, can be absorbed in the normalization constant \mathcal{N}' , and are thus irrelevant. This allows us to parametrize the most general Thouless pair expressed in Eq. (1) in terms of two angles $0 \leq \alpha < \pi$ and $0 \leq \varphi < \pi$ only, that is, $\hat{Z}^+(p_0, d_0) \equiv \hat{Z}^+(\alpha, \varphi)$ for

$$p_0 = \sin(\frac{1}{2}\alpha) e^{-i\varphi} \quad \text{and} \quad d_0 = \cos(\frac{1}{2}\alpha) e^{i\varphi}. \quad (5)$$

The angle α (φ) controls the relative amplitude (phase) between the isovector and isoscalar pairs.

Third, we have to take into account the fact that every scalar and isoscalar Hamiltonian is also invariant with respect to the spin and isospin signatures, $\hat{S} \equiv \exp(i\pi \hat{S}_y) = i\hat{\sigma}_y$ and $\hat{T} \equiv \exp(i\pi \hat{T}_y) = i\hat{\tau}_y$, respectively, which rotate spins and isospins by angle π about the corresponding y axes. Transformation rules of the isovector and isoscalar pairs under such rotations follow directly from the general rules of how scalars and vectors are transformed. Indeed, any scalar is invariant with respect to the rotation by angle π , and any vector then changes sign. It thus follows that the scalar pairs are S -even- T -odd and the isoscalar pairs are S -odd- T -even, and thus the Thouless pairs (1) transform as:

$$\hat{S} \hat{Z}^+(\alpha, \varphi) \hat{S}^+ = i \hat{Z}^+(\alpha, \varphi + \frac{\pi}{2}), \quad (6)$$

$$\hat{T} \hat{Z}^+(\alpha, \varphi) \hat{T}^+ = i \hat{Z}^+(\alpha, \varphi - \frac{\pi}{2}). \quad (7)$$

Finally, we have to fix the phase convention. Here we adopt the one of Condon-Shortley in the LS basis, by which all single-particle states transform under time-reversal \hat{T} as,

$$\hat{T} a_{\ell m; \frac{1}{2} s_z; \frac{1}{2} t_z}^+ \hat{T}^+ = (-1)^{\ell+m} (-1)^{\frac{1}{2}+s_z} a_{\ell -m; \frac{1}{2} -s_z; \frac{1}{2} t_z}^+. \quad (8)$$

This convention carries over to the isovector and isoscalar pairs, Eqs. (3) and (4), which turn out to be time-even and time-odd, respectively. As a consequence, the Thouless pairs transform under time reversal as

$$\hat{T} \hat{Z}^+(\alpha, \varphi) \hat{T}^+ = i \hat{Z}^+(\alpha, \frac{\pi}{2} - \varphi). \quad (9)$$

Altogether, we see that the invariance of the Hamiltonian with respect to the spin or isospin signature renders the average energies periodic in φ with period of $\frac{\pi}{2}$, whereas that with respect to the time reversal renders them symmetric with respect to the line

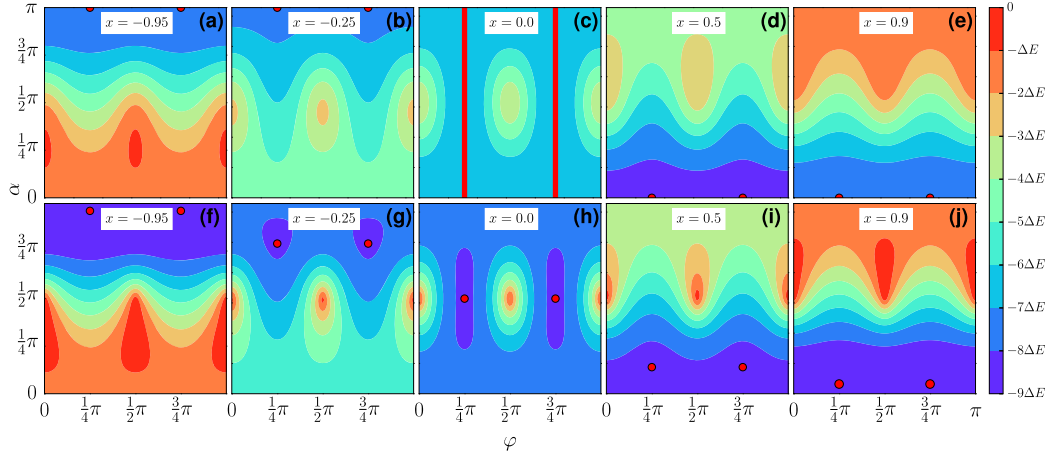


Fig. 1. Average values of the SO(8) Hamiltonian (10), calculated for the unprojected (upper panels) and projected (2) (lower panels) Thouless states, parametrized by angles α and φ as in Eqs. (1) and (5). Calculations were performed for $\Omega = 12$, with projection on $A = 24$ and $T = S = 0$. From left to right panel we show results for $x = -0.95, -0.25, 0, 0.5$, and 0.9 , and color bands correspond to steps of $\Delta E = 20, 15, 13, 17$, and 20 , respectively. All results are in units of g .

at $\varphi = \frac{\pi}{4}$. At this line, the Thouless pairs are time-even (up to an irrelevant phase factor).

Since our entire analysis of symmetries is performed for the Thouless states, we avoid any possible ambiguities related to definitions and phase conventions of quasiparticle states, density matrices, and pairing tensors, which can be now consistently determined from the Thouless pairs using generic expressions [8].

For the Hamiltonian of the SO(8) model we use the representation introduced in Ref. [21],

$$\hat{H} = -g(1-x) \sum_{\nu=0,\pm 1} \hat{P}_\nu^\dagger \hat{P}_\nu - g(1+x) \sum_{\mu=0,\pm 1} \hat{D}_\mu^\dagger \hat{D}_\mu. \quad (10)$$

The model makes it possible to study the dynamical properties and relative importance of the isoscalar and isovector modes of pairing. Indeed, with the overall pairing strength controlled by parameter g , the relative importance of the isovector vs. isoscalar pairing is governed by the mixing parameter x . For $x = +1(-1)$, the Hamiltonian has a pure isoscalar (isovector) character, whereas within the interval $-1 < x < 1$, we should expect a competition between the two possible types of pairing. Using group-theory methods the Hamiltonian, specified by Eq. (10), can be diagonalized exactly [17, 21].

In Fig. 1, we show average values of the SO(8) Hamiltonian (10) calculated for the unprojected Thouless states (upper panels) and for Thouless states projected for particle number $A = 24$ and $T = S = 0$ (lower panels). The red dots and red band indicate the minima of energies, that is, in the upper and lower panels they indicate solutions of the HFB and VAP equations, respectively. We see that in all cases the minima of energies appear at $\varphi = \frac{\pi}{4}$, that is, for time-even Thouless states.

For the unprojected states, for $x < 0$ the minima stay at $\alpha = \pi$ (purely isovector pairs) and then for $x > 0$ they flip over to $\alpha = 0$ (purely isoscalar pairs). At $x = 0$, the HFB energy is entirely independent of α , so that states with any isovector-isoscalar pair mixing are exactly degenerate. Our HFB results confirm the observations of Ref. [19] that the unprojected mean-field states do not exhibit isovector-isoscalar pairing mixing. However, as we see in the lower panels of Fig. 1, our VAP states do exhibit such a mixing. Indeed, even a small departure from the pure isovector or isoscalar interaction moves the VAP solutions away from the unmixed states characterized by $\alpha = 0$ or $\alpha = \pi$. As expected, at $x = 0$ the VAP solution appears at $\alpha = \frac{1}{2}\pi$, so that the pairs are then maximally mixed.

Let us now discuss the VAP solutions, that is, properties of states $|AST\rangle$ that are projected on good particle number A , spin S , and isospin T with energies minimized over α at $\varphi = \frac{\pi}{4}$. Fig. 2 summarizes our VAP results obtained for different isospins (left panels) and particle numbers (right panels).¹ As one can see in the top panels of the figure, when plotted on a linear scale, the VAP energies (symbols) are indistinguishable from the exact values (lines).

Only by plotting energy differences on a logarithmic scale (upper middle panels) can one appreciate the fact that at $x = 0$ the VAP energies are precise up to 1.5%, and that with growing $|x|$ their precision rapidly improves by many orders of magnitude. In the limits of $x = -1$ or $x = +1$, the Thouless pairs correspond to $S = 0$ or $T = 0$, respectively, and thus it is enough to restore either the isospin or spin symmetry. Then, as already noted in Ref. [20], the VAP results become exact. Here we have shown that even in a more realistic case of mixed pairing the VAP results constitute an excellent approximation to the exact ones. We also note that for the multi-level $T = 1$ pairing model very good results were obtained in Ref. [23] by using the GCM mixing of the isospin-restored HFB states, with pairing gaps used as generator coordinates. In light of our findings, one can interpret such a GCM approach as leading to analogous solutions to those that we obtain by employing the full VAP method. Finally, as one can see in Fig. 2(d), the VAP results obtained for $A = 4$ and 6 are for all values of x exact, that is, precise up to the numerical accuracy, see discussion below.

The lower middle panels of Fig. 2 show norms of the VAP Thouless isoscalar pairs defined as $|d_0|^2 = \cos^2(\frac{1}{2}\alpha_{\min})$, cf. Eqs. (1) and (5). Again we see that for arbitrary strengths of the isoscalar vs. isovector interactions, the VAP isoscalar and isovector pairs do coexist. As illustrated in Fig. 2(e), at a given interaction strength $x > 0$, the role of the isoscalar pairs gradually decreases with isospin T , however, even for high values of T their contributions are still significant.

A possible experimental evidence of coexistence between isoscalar and isovector pairing can be the observation and analysis of deuteron transfer reaction [24–26], which depends on the reduced isoscalar-pair transfer matrix element $\langle A+2, S=1, T||D^+||A, S=0, T\rangle$. In the bottom panels of Fig. 2, we compare the VAP and exact values of these matrix elements calculated in the SO(8) model. Here we show results normalized by the maximum values ob-

¹ We plot VAP results only for projected states $|AST\rangle$ that have numerically significant norms.

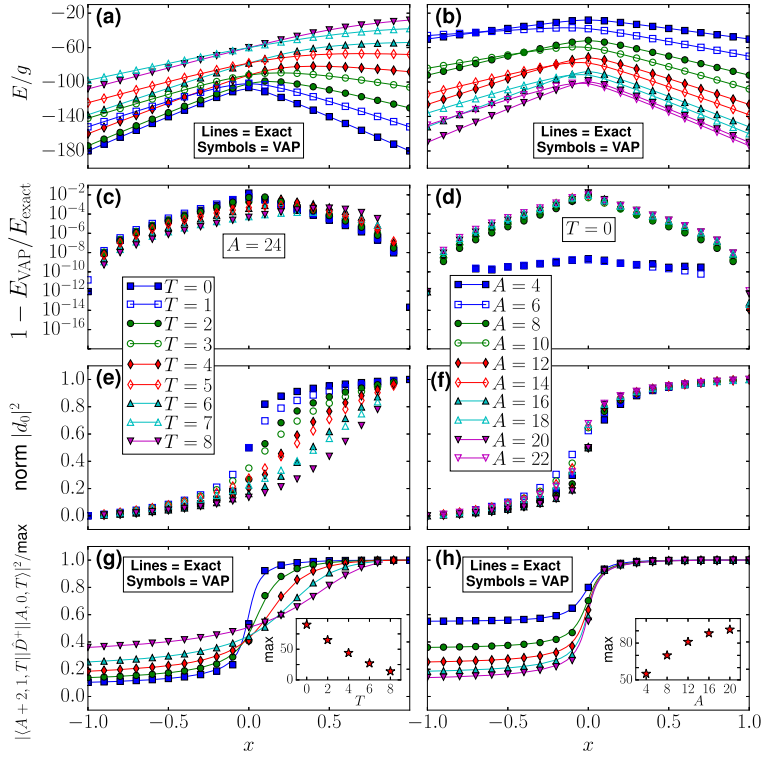


Fig. 2. Top panels: Energies in units of g . Upper middle panels: Relative errors of the VAP energies shown in the logarithmic scale. Lower middle panels: Norms of the isoscalar Thouless pairs $|d_0|^2$. Bottom panels: Deuteron-transfer matrix elements. In the top and bottom panels, results obtained within the VAP method (symbols) are compared with those corresponding to the exact solutions (lines). Left panels show results obtained for $A = 24$, with the isospin increasing from $T = 0$ to 8, and spin $S = 0$ or 1 for even and odd T , respectively. Right panels show results obtained for $T = 0$, with the particle number increasing from $A = 4$ to 22, and spin $S = 0$ or 1 for even and odd $A/2$, respectively.

tained at $x = 1$, whereas the insets show these maximum values plotted in the absolute scale. Again we see that the VAP results (symbols) are indistinguishable from the exact values (lines).

On the one hand, the relative deuteron transfer amplitudes increase with the strength of the isoscalar interaction, but this increase is fairly gradual, especially at higher isospins. On the other hand, absolute values of these amplitudes gradually decrease with the isospin. So, as expected, the observation of the strong deuteron transfer is most likely in $N = Z$ nuclei, however, for $N \neq Z$, the effect does not abruptly disappear. The $SO(8)$ model is too simplistic to draw quantitative conclusions and an analysis performed in a realistic shell-structure setting is very much required.

The fact that the projected pair condensates properly describe isovector and isoscalar pairing correlations can be best seen by analyzing the simplest case of four particles. Then, the particle-number projected condensate is given by the square of the Thouless pair (1), that is, by $|\Phi_4\rangle = \mathcal{N}(\hat{Z}^+)^2|0\rangle$. However, the square of the Thouless pair is equal to a linear combination of five quartets: $(P^+P^+)^{(00)}$, $(D^+D^+)^{(00)}$, $(P^+D^+)^{(11)}$, $(P^+P^+)^{(02)}$, and $(D^+D^+)^{(20)}$, where superscripts (ST) denote values of the total spin S and isospin T . Restoration of the spin and isospin symmetries corresponds in this case to keeping only the first two, scalar-isoscalar quartets, and removing the other three. Thus the symmetry-projected $|AST\rangle = |400\rangle$ state becomes an exact linear combination of the two basic quartets [27]. Similarly, the symmetry-restored state $|610\rangle$ corresponds to an exact linear combination of these same two basic quartets supplemented by one vector-isoscalar pair D^+ (4). As a result, the $A = 4$ and 6 VAP solutions shown in Fig. 2(d) are identical to the exact ones. For larger particle numbers or isospins, the success of the VAP approach in describing the pair condensation relies on the fact that it properly

accounts for the main components of the wave functions being given by the two basic scalar-isoscalar quartets.

We note here that the pn pairing models have already been intensely analyzed within the quartet-condensation models, see Refs. [27,28] and references quoted therein. These references have often compared results with those obtained within pair-condensation models employed without full VAP symmetry restorations and concluded that the latter ones were inferior. At variance with those conclusions, our results show that the obtained inferiority was not related to the pair-condensate approximation itself, but rather to the lack of the full VAP symmetry restoration. We stress that approaches aiming to mix the isovector and isoscalar pairing necessarily mix the isovector ($T = 1$) and vector ($S = 1$ or $J = 1$) pairs, and thus a *simultaneous* restoration of isospin and angular momentum is mandatory [29].

It is now obvious that the effects of the pn-pair condensation should be analyzed in a more sophisticated setting than that envisaged up to now. Within a mean-field approach, it appears that only by performing the VAP calculations one can fully account for a subtle balance between the isovector and isoscalar pairing correlations.

Methods to obtain full VAP results for realistic density functionals have already been formulated [30], and implemented [31], in the simplest case of the particle-number restoration. When combined with the full restoration of rotational and isospin symmetries, which were implemented without pairing in Ref. [32], and with the seven-dimensional symmetry restoration implemented in this Letter, a complete approach is possible and is now being constructed.

For the Coulomb isospin mixing included together with pairing, a reduction of the three-dimensional isospin restoration to one dimension is not possible. Moreover, the former will anyhow

be required if the isocranking technology [10,11,33,34] is used to control the isospin degree of freedom. However, for axial nuclei, a one-dimensional integration suffices, so altogether we are then faced with five-dimensional integrals – which is a fully manageable task. Before attacking the full VAP approach, the results of this Letter indicate that a restricted minimization of the projected energies with respect to relative amplitudes of the isovector and isoscalar pairs could be a viable simplifying option.

The possibility of implementing such a methodology in a realistic setting of microscopic density functionals crucially depends on developing functionals based on density-independent generators [35] with controlled isoscalar vs. isovector pairing strengths. We have already implemented the second aspect by adding to the inventory of generators terms separable in the pairing channel, cf. Refs. [36–39]. The work towards obtaining functionals suitable for the full VAP treatment of the pn pairing is now being intensely pursued.

In conclusion, within a simple $SO(8)$ pairing model, we have shown that the symmetry-projected condensates of mixed isovector and isoscalar pairs very accurately describe properties of the exact solutions, including the coexistence of the isovector and isoscalar pairing. Lack of symmetry restoration thus explains the limited success in describing such a coexistence in the standard mean-field approaches to date. Symmetry restoration is also key to reconciling the pair-condensation and quartet-condensation pictures of paired systems. Our study suggests that further work on properties of the proton-neutron nuclear pairing should be, and can be, carried out within the variation-after-projection approach to mean-field pairing methods.

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